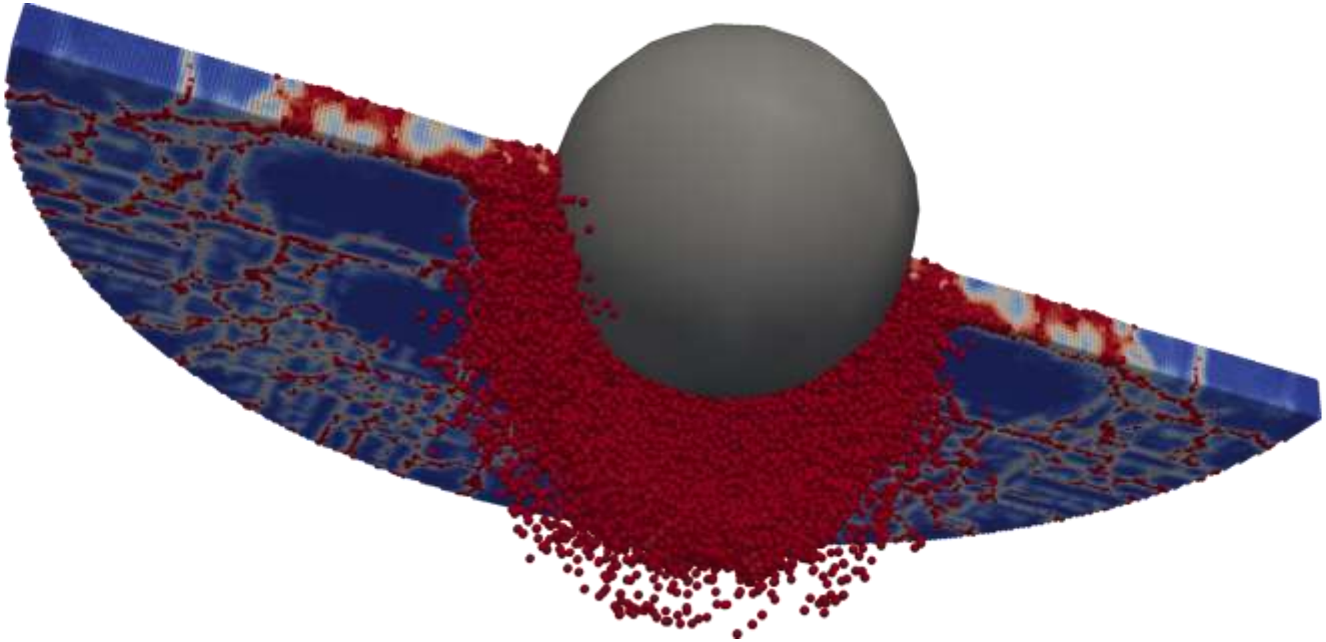
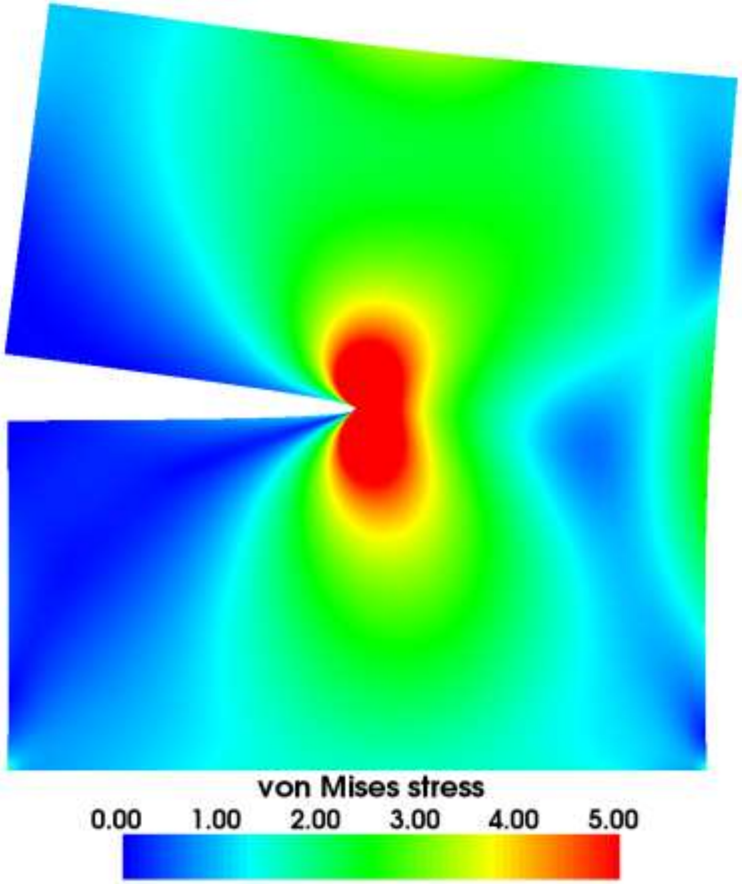
D.7
Meshfree Multiscale Methods for Solids

Marc Alexander Schweitzer
Sa Wu





Particle Methods

Pros

- Very accurate
- Well studied
- Physically meaningful
- Expert knowledge included
- …

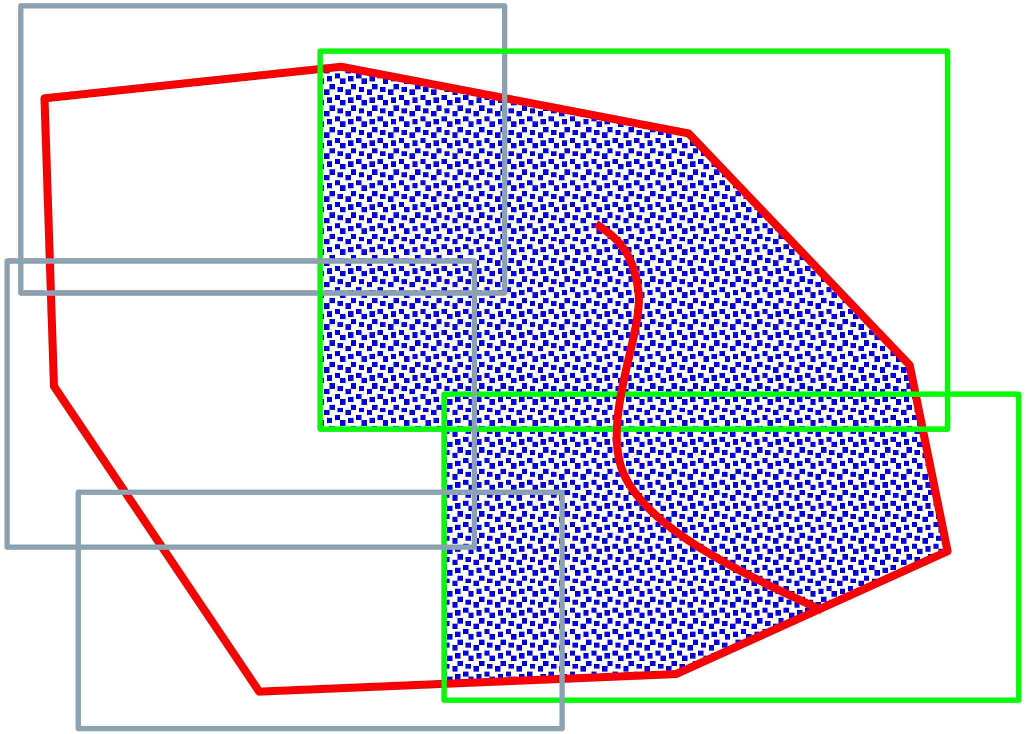
Cons

- Everything only for small samples

What to do?

- Particles only where needed
  - Coupling?

Idea



Smooth, coarse scale Method

- e.g. Finite Elements

Discontinuous, fine scale Method

- e.g. Molecular Dynamics

Together

1. Detect areas where fine scale important
2. Fine scale simulations to obtain local solutions
3. Build additional basis function from local solutions
4. Compute global solution including function from Step 3
5. Use global solution for Steps 1, constraints of Step 2

Peridynamics

Classical Elasticity

- Partial Differential Equation of Motion

$$\rho\ddot{u}(x,t) = f(x, u(x,t), \nabla u(x,t), \nabla^2 u(x,t)) + b(x,t)$$

- Spatial derivatives

$$\nabla u(x,t), \qquad \nabla^2 u(x,t)$$

Peridynamic Model

- Nonlocal Equation of Motion ($\Omega(x)$ finite size)

$$\rho\ddot{u}(x,t) = \int_{\Omega(x)} f(\underbrace{y-x}_{\xi}, \underbrace{u(y,t)-u(x,t)}_{\eta})\, dy + b(x,t)$$

- No gradients, but differences in finite distance $\Omega(x)$

$$\xi = y - x, \qquad \eta = u(y,t) - u(x,t)$$

- Particle discretization

$$\rho\ddot{u}(x_i, t_n) = \sum_{x_j \in \Omega(x_i)} f(x_j - x_i, u(x_j, t_n) - u(x_i, t_n)) V_{i,j} + b(x_i, t_n)$$

[Silling, Parks, Weckner et al.]

Peridynamic material description

Integration domain

- $\Omega(x), N(x_i)$

Pairwise force function

- $f(\xi,\eta)$
- Preservation of linear and angular momenta

$$f(-\xi,-\eta) = -f(\xi,\eta), \qquad f(\xi,\eta)\times(\xi+\eta) = 0$$

- Example
  - Isotropic

$$f(\xi,\eta) = \underbrace{g(\xi,\eta)}_{\text{scalar}}\frac{\xi+\eta}{\|\xi+\eta\|}$$

  - Prototype Microelastic

$$g(\xi,\eta) = g(\underbrace{\frac{\|\xi+\eta\|-\|\xi\|}{\|\xi\|}}_{s}) = \begin{cases} cs, & \forall\tilde{t}\leq t: s\leq s_0 \\ 0, & \text{otherwise} \end{cases}$$

  - Breakable linear springs
- Many more

Peridynamics

Theoretical Results

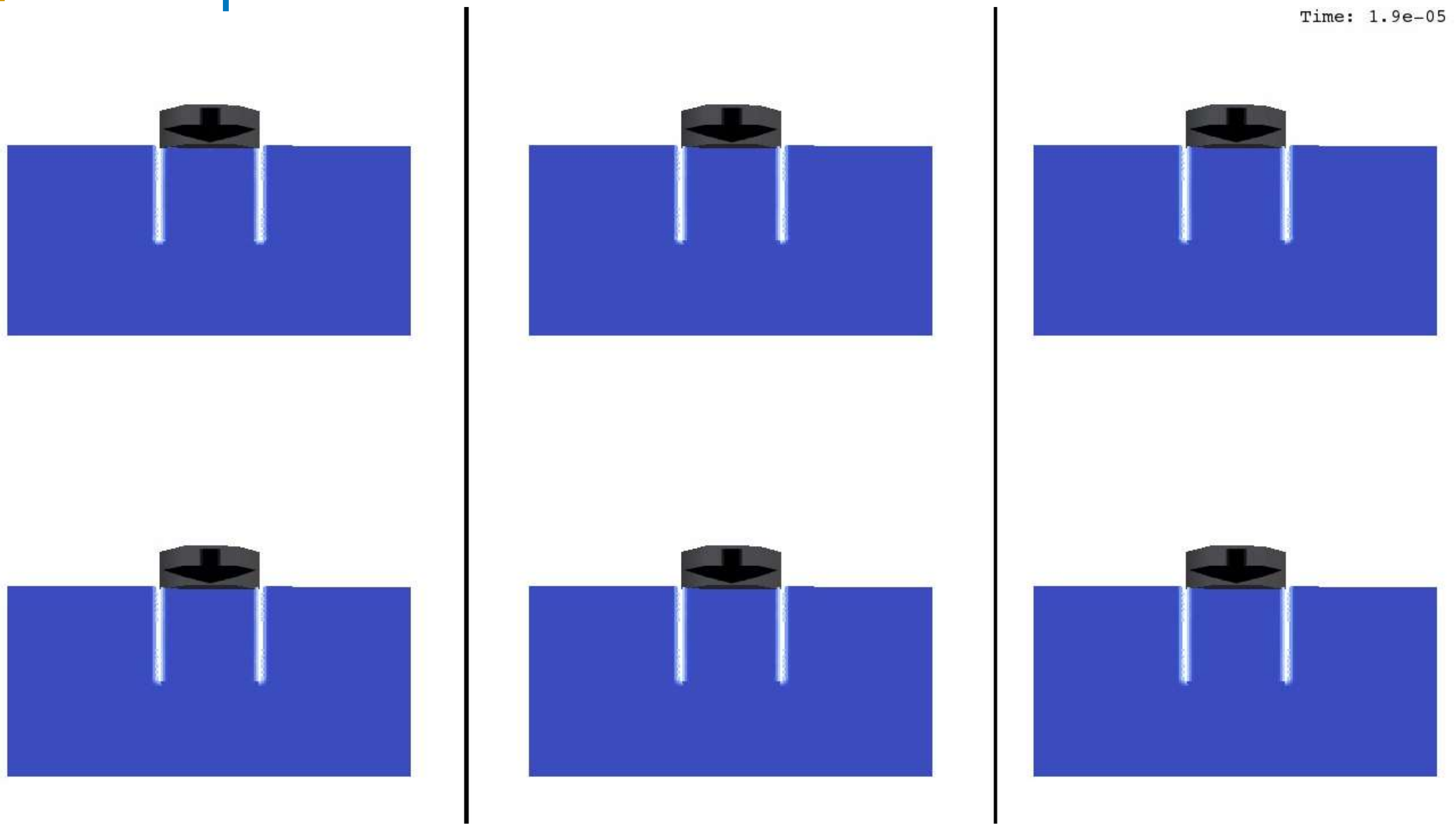
- Linear Elasticity:
  Linear kernel with certain properties, for $\delta = \max_x \operatorname{diam}(\operatorname{supp}(\Omega(x))) \rightarrow 0$:
  Convergence Navier equation of linear elasticity

  [Emmrich & Weckner, Silling & Lehoucq]

- Molecular Dynamics:
  - Peridynamics and MD result in “same” HOG model
  - Can build PD kernel from MD potential

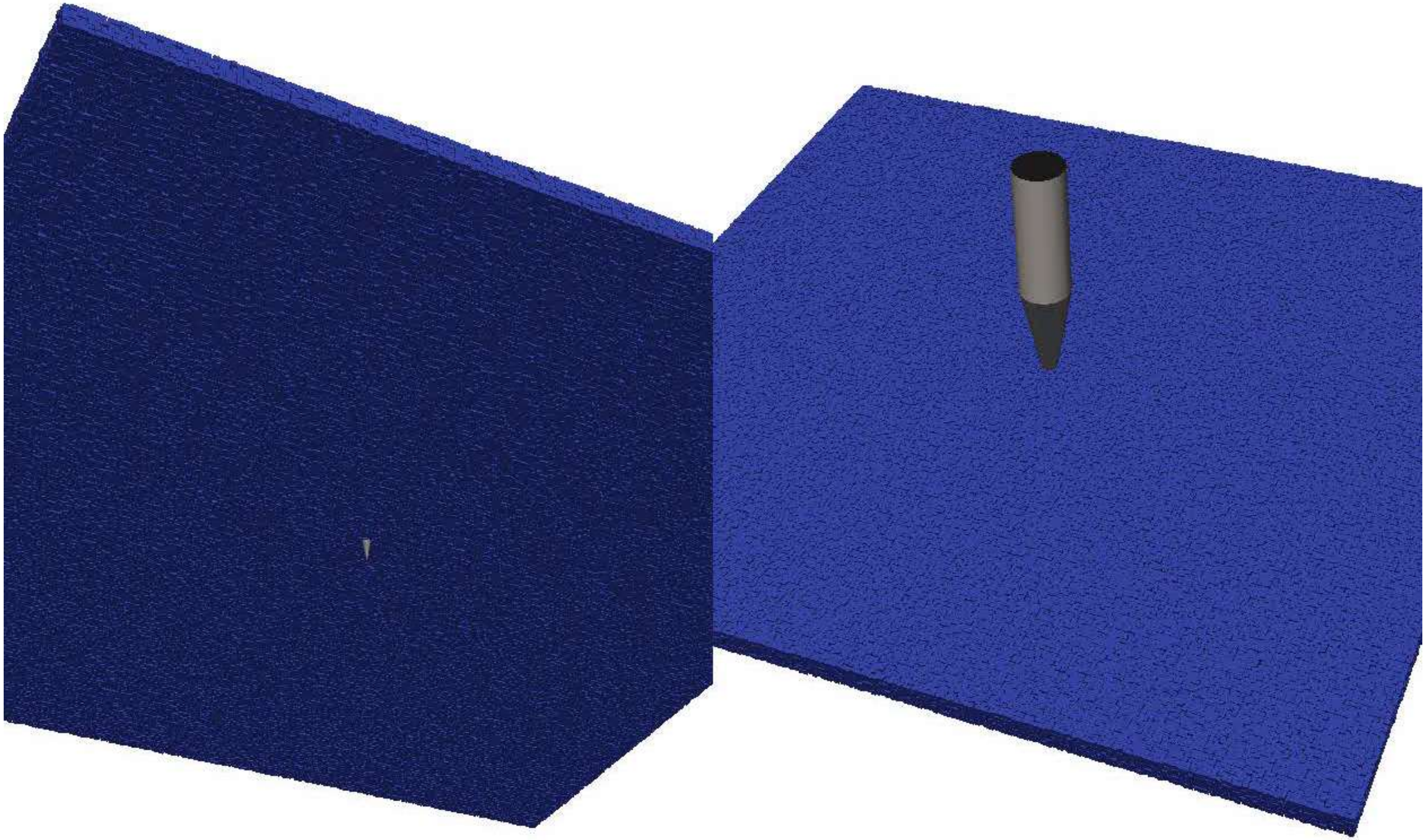
  [Seleson & Parks & Gunzburger & Lehoucq]

Examples



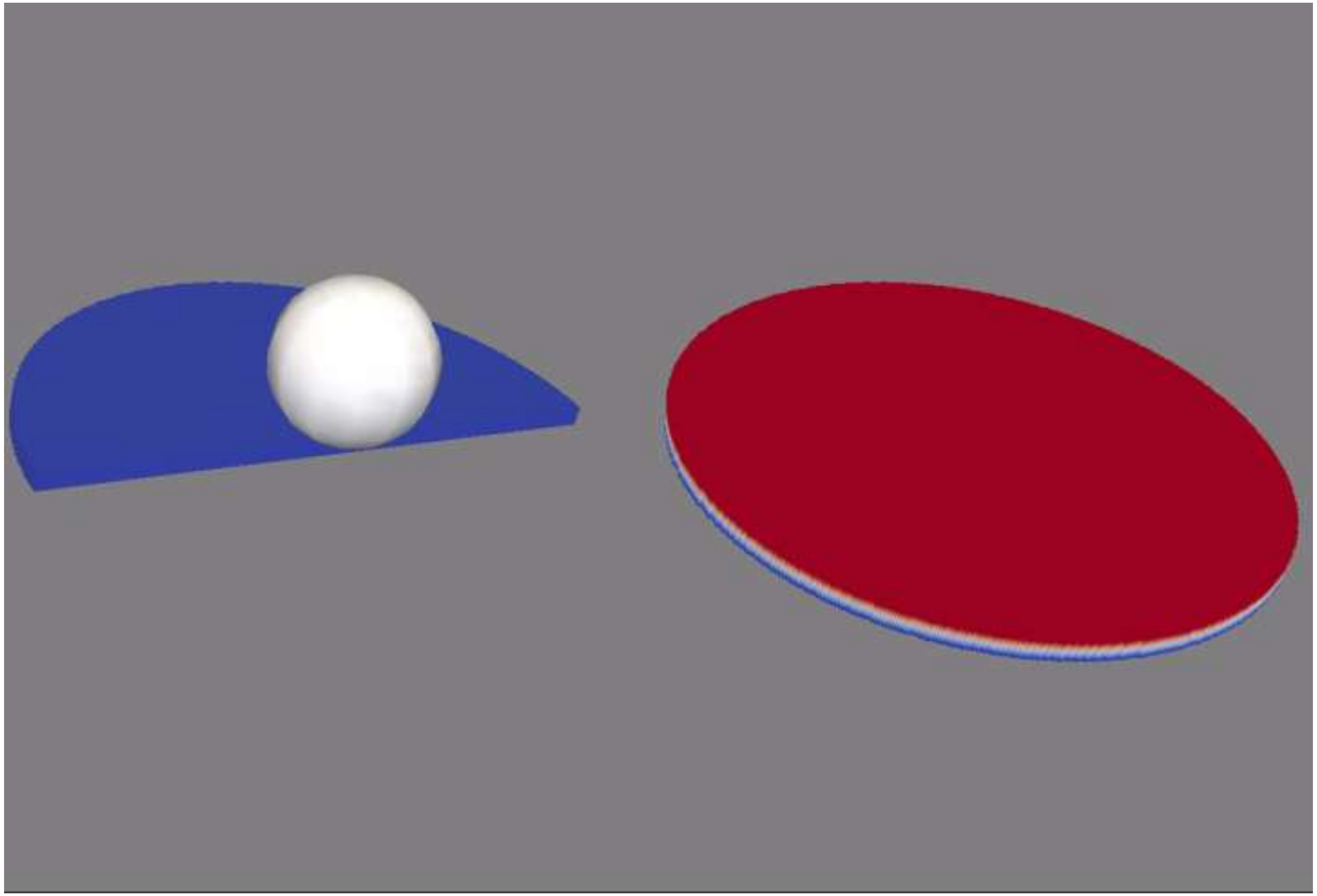
Peridynamics simulation of the Kalthoff-Winkler experiment for varying material parameters
10000 time steps à $10^{-8}\mathrm{s}$ with 178000 particles à $1\mathrm{mm}^3$

Examples



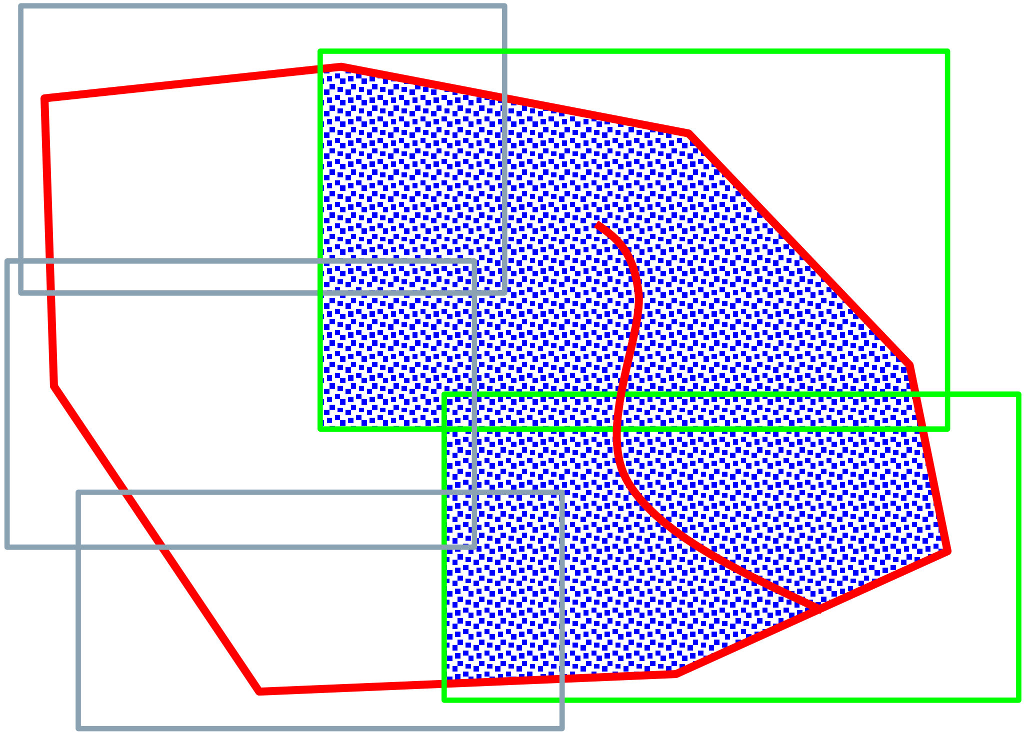
Peridynamics simulation of impact scenario
3000 time steps à 10^{-4}s with 200000 particles à 1mm^3

Examples



Peridynamics simulation of impact scenario
10000 time steps à 10^{-8}s with 13144032 particles à 0.25mm^3

Idea



Smooth, coarse scale Method

- e.g. Finite Elements

Discontinuous, fine scale Method

- Particle discretization of Peridynamics

Together

1. Detect areas where to use particles x_i
2. Peridynamics simulation with x_i obtain $(x_i, u_i = u(x_i, t))$
3. Build additional basis function $\tilde{u}$ from (x_i, u_i)
4. Compute global solution u with $\tilde{u}$ as additional basis function
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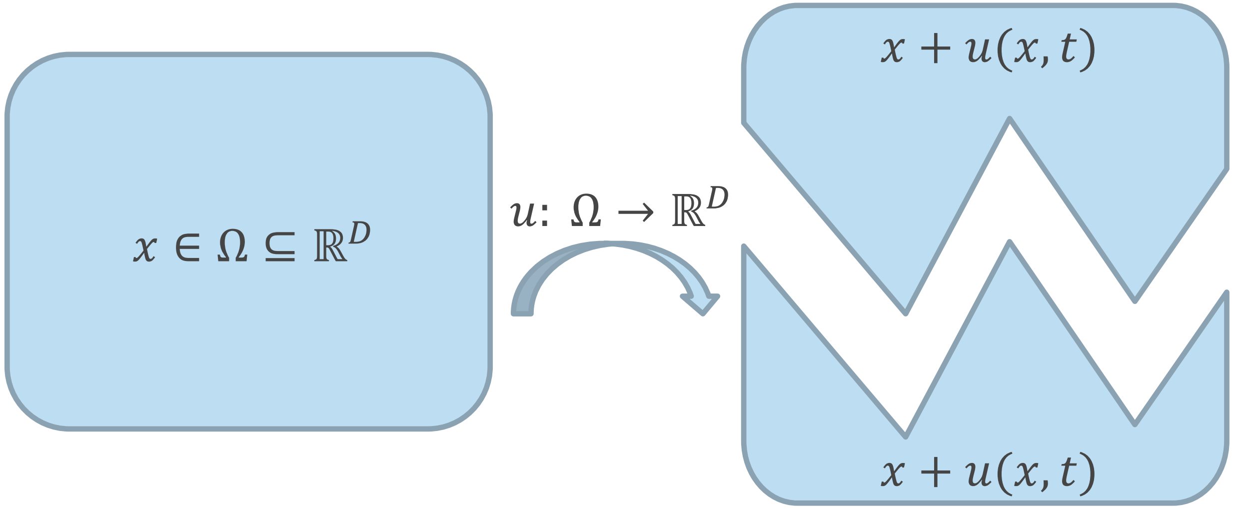
Decomposition of

Smooth displacements

- Partial Differential Equations
  - e.g. Finite Elements
  - Cheap
  - Large Samples



Discontinuous displacements

- Material failure
- Crack nucleation and growth
- Equations where spatial regularity not needed
  - e.g. Molecular Dynamics, Peridynamics
  - Expensive
  - Small Samples

Decomposition of Solution

- Behavioural Decomposition:

$$u = u_{\text{smooth}} + u_{\text{jump}} + u_{\text{singular}}$$

- Partition of Unity:

$$\varphi_i, \omega_i = \text{supp}(\varphi_i)$$

- Localized Decomposition:

$$u = \sum_i \varphi_i \left(u_{\text{smooth}} + u_{\text{jump}} + u_{\text{singular}} \right)\Big|_{\omega_i}$$

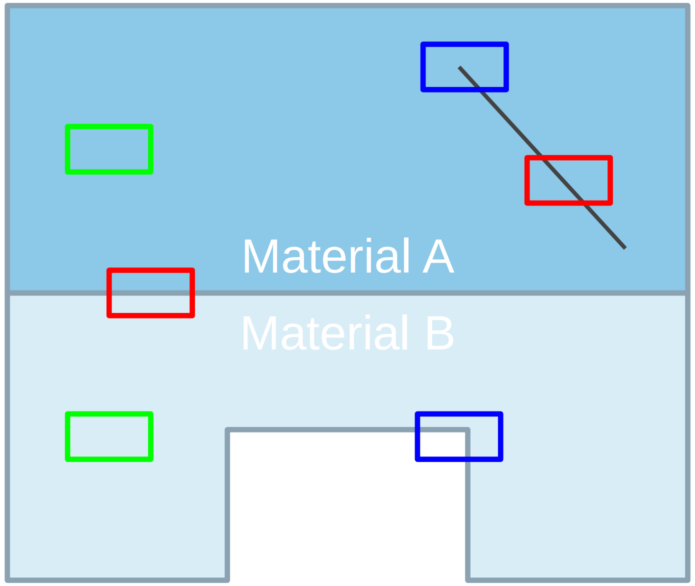
- Localization of Approximation:

$$u\Big|_{\omega_i} \approx u^i \in V^i(\omega_i)$$

- Smooth Splicing of Local Spaces

$$V = \sum_i \varphi_i V^i(\omega_i) = \sum_i \varphi_i \left(P^i + \mathcal{E}^i \right)$$

$$u = \sum_i \varphi_i u\Big|_{\omega_i} = \sum_i \varphi_i \left(\overbrace{u_{\text{smooth}}\Big|_{\omega_i}}^{\wr\wr} + \overbrace{u_{\text{jump}}\Big|_{\omega_i} + u_{\text{singular}}\Big|_{\omega_i}}^{\wr\wr} \right)$$



Enrichments

Scenario

- Exact
  - Known Singularity
  - Known Discontinuity
- Approximate, Asymptotic
  - Singularity
  - Discontinuity
  - Boundary layers
  - Radial component
- Numerical
  - Eigenfunctions of local problems
  - Reconstruction of experimental data
  - Local fine scale solution

Examples

$$\eta(x) = \|x - x_0\|^{\alpha}$$

$$\eta(x) = \cos\left(\frac{\theta}{2}\right)$$

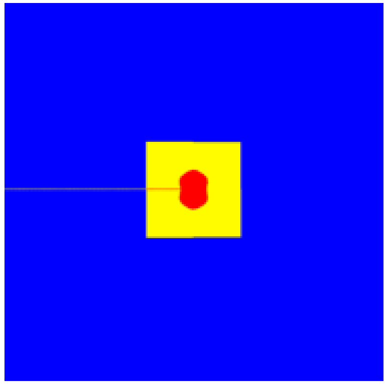
$$\eta(x) = \|x - x_c\|^{\beta}$$

$$\eta(x) = H_{\pm}(x - c)$$

$$\eta(x) = \exp(1 - \mathrm{dist}(x, c))$$

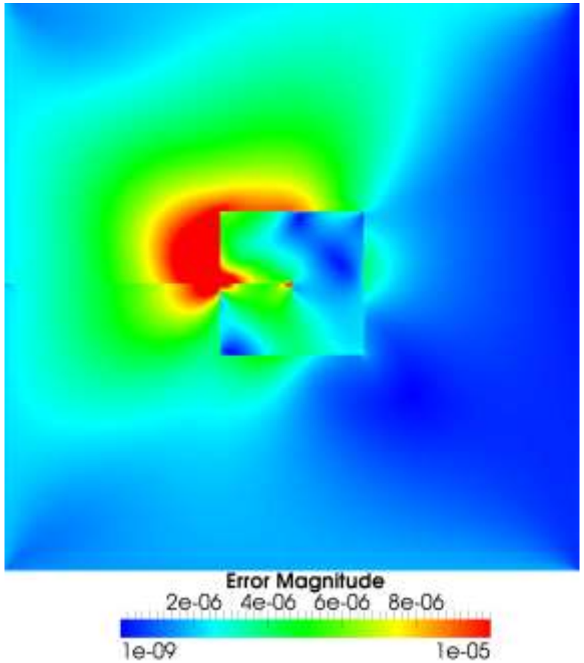
Partition of Unity Method

- Finite Elements to solve local $u|_{\omega_i} \approx u^i \in V^i(\omega_i)$
- Example
  - Linear Fracture Mechanics
  - Exact solution:
  - across crack



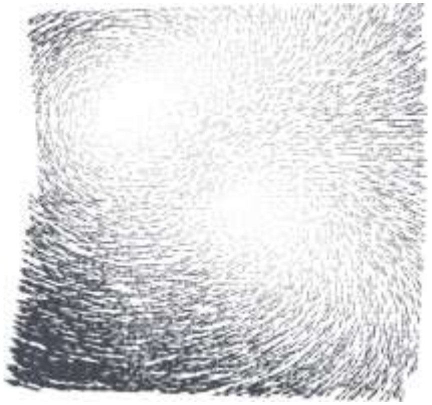
$$\mathcal{E} = P^i \cdot H^C$$

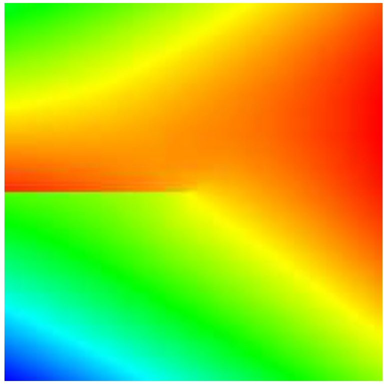
enrichment



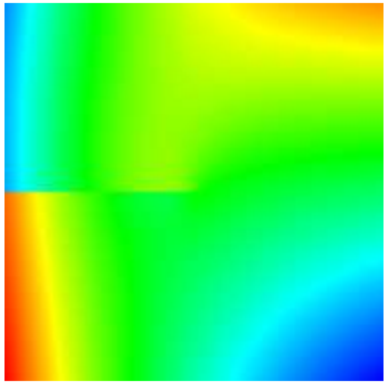
  - Crack tip

$$\mathcal{E} = \left\{\sqrt{r}\cos\frac{\theta}{2}, \sqrt{r}\sin\left(\frac{\theta}{2}\right), \sqrt{r}\sin\theta\sin\frac{\theta}{2}, \sqrt{r}\sin\theta\cos\frac{\theta}{2}\right\}$$



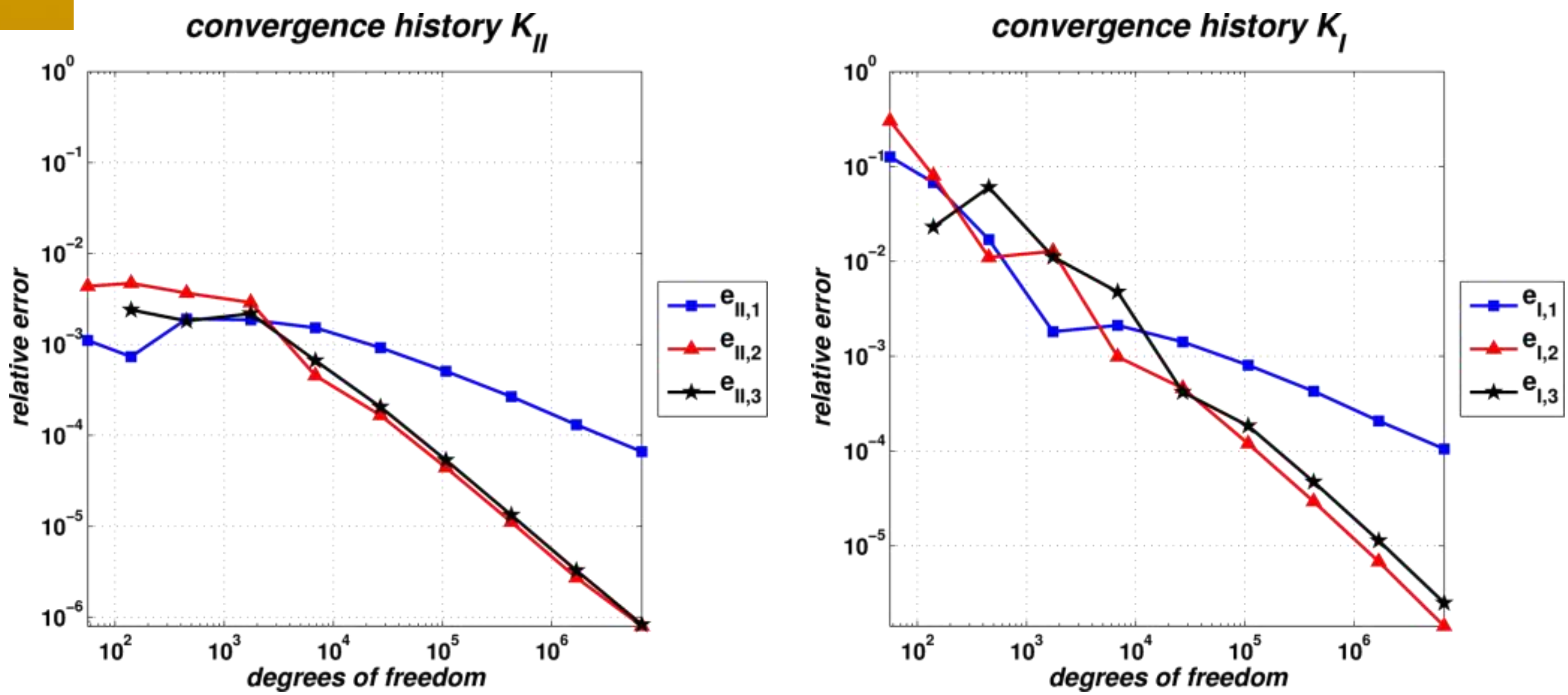


x – component



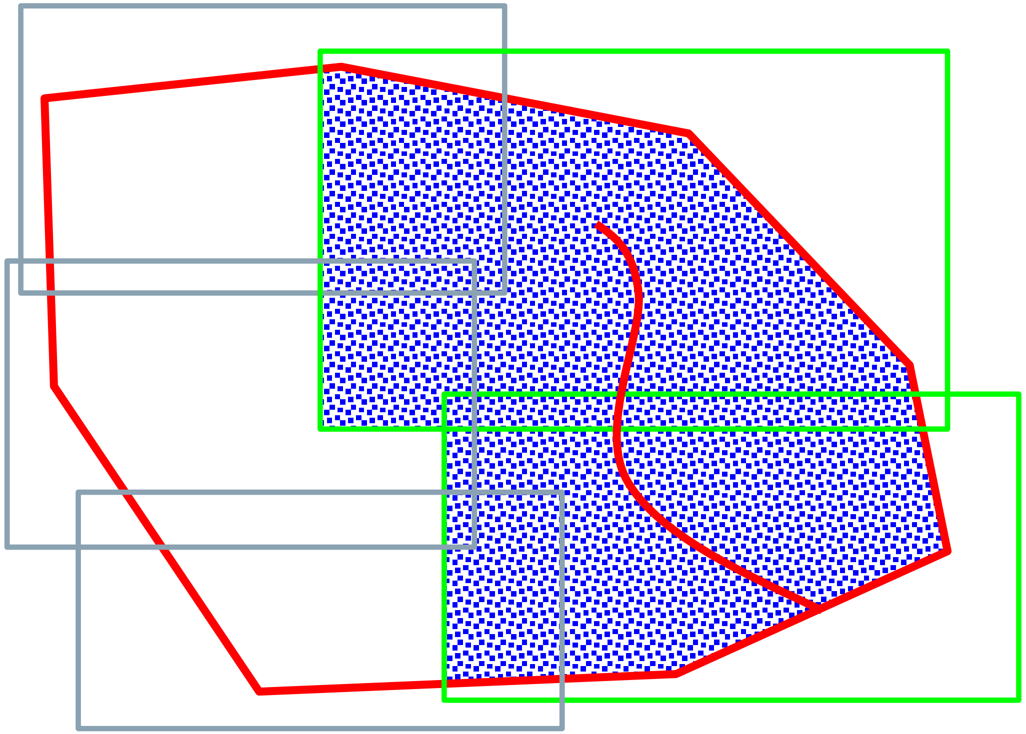
y – component

[Babuška, Melenk, Belytschko et. al]



Convergence of stress intensity factors for $[-0.5, 0.5]^2$, $[-0.25, 0.25]^2$, $[-0.125, -0.125]^2$

Idea



Smooth, coarse scale Method

- Partition of Unity Method

Discontinuous, fine scale Method

- Particle discretization of Peridynamics

Together

1. Detect areas where to use particles x_i
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Construction of Enrichment

- Have, Assume to get
  - Data points $x_i \in \Omega \subseteq \mathbb{R}^3$
  - Displacements $u_i = u(x_i, t) \in \mathbb{R}^3$
  - Adjacency $A_{i,j} = \begin{cases} 1, & x_i, x_j \text{ connected} \\ 0, & \text{otherwise} \end{cases}$

- Want
  - Piecewise smooth
  - Possibly discontinuous
  - Easy to integrate.
  - Easy to get derivatives
  - …

Moving Least Squares

Scattered Data Approximation

- Find approximation p to arbitrary data points (x_i, u_i)

Least Squares

- Find

$$p = \underset{q \in V}{\operatorname{argmin}}\, J(q) = \sum_i (u_i - q(x_i))^2$$

- Get approximation $\mathrm{p} \in V$

Moving Least Squares

- Find for each x

$$p(x) = \underset{q \in V}{\operatorname{argmin}}\, J_x(q) = \sum_i W_i(x)(u_i - q(x_i))^2$$

- Get approximation $p \notin V$

[Shepard, Farwig, Belytschko, Wendland et al.]

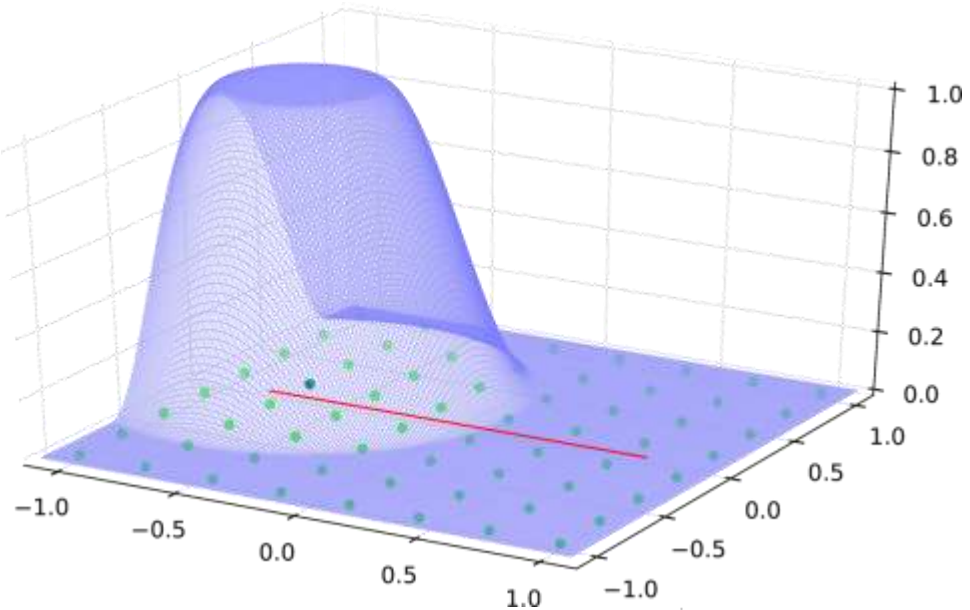
Moving Least Squares

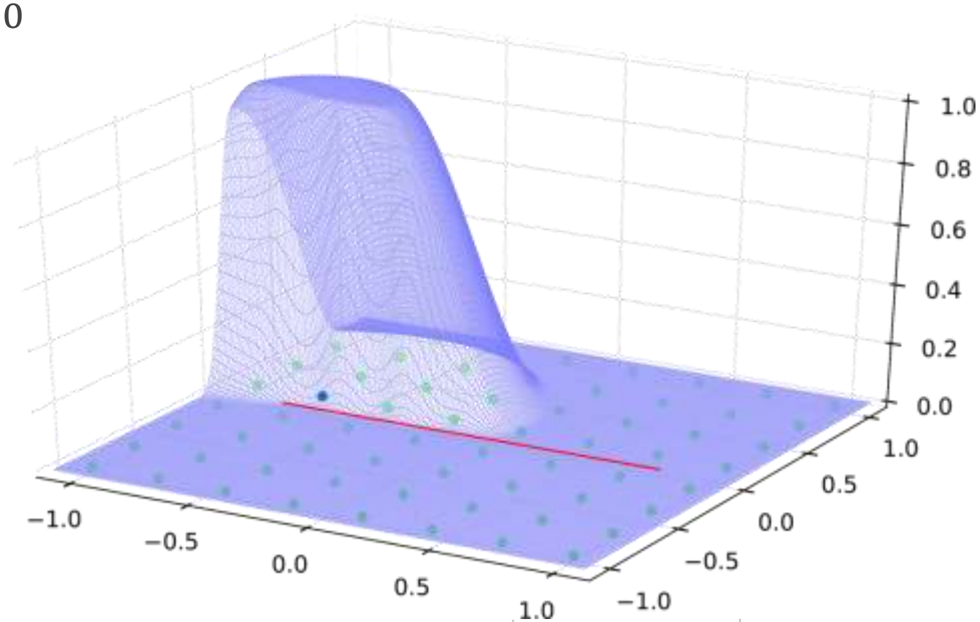
- $0 \leq W_i(x)$: how important error at x_i for evaluation in x
  - Gaussians, Splines in Radial or Tensor structure

- Put adjacency $A_{i,j}$ into weights:

$$0 \leq w_i \leq 1, \qquad w_i\Big|_{B_\epsilon(x_i)} \equiv 1, \qquad \min_{j:A_{i,j}=1} \|x_i - x_j\| \leq \operatorname{diam}(\operatorname{supp}(w_i))$$

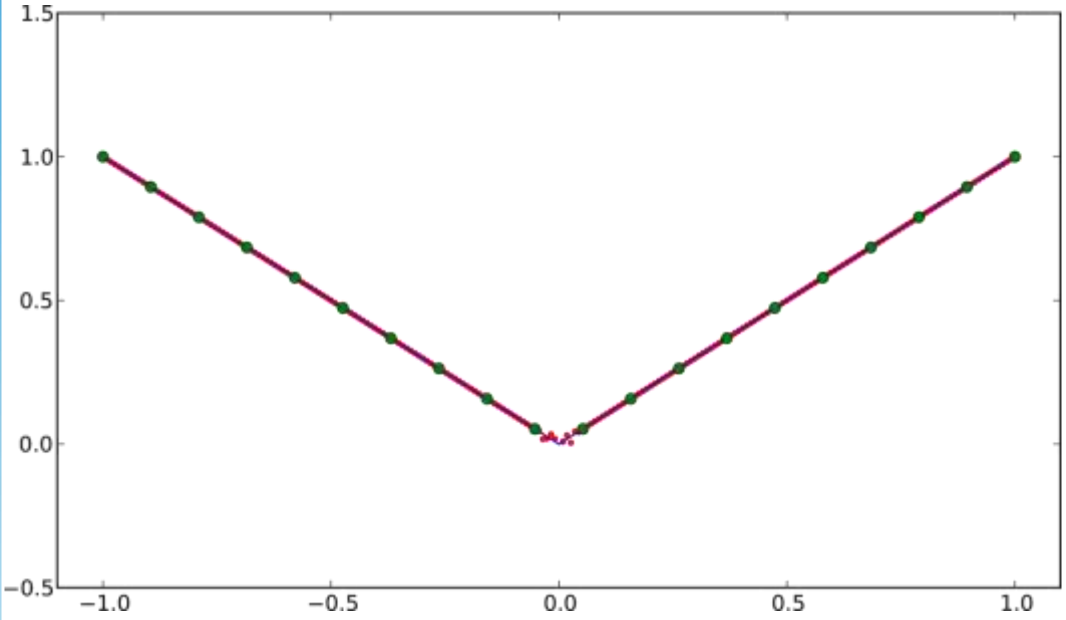
$$\widetilde{W}_i(x) = W_i(x) \prod_{j:A_{i,j}=0} (1 - w_j(x))$$

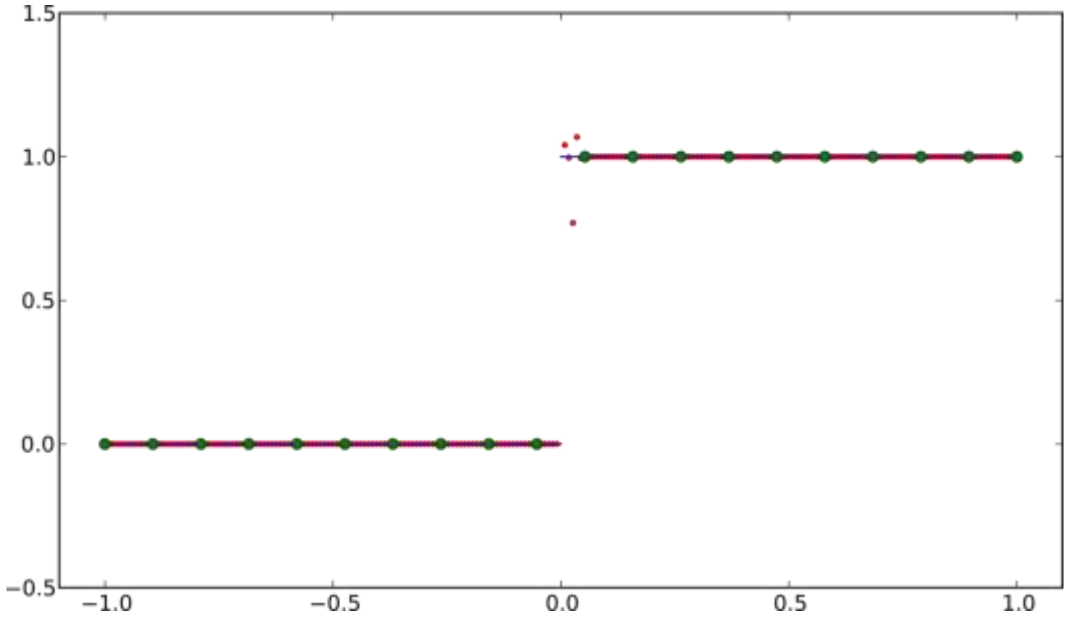


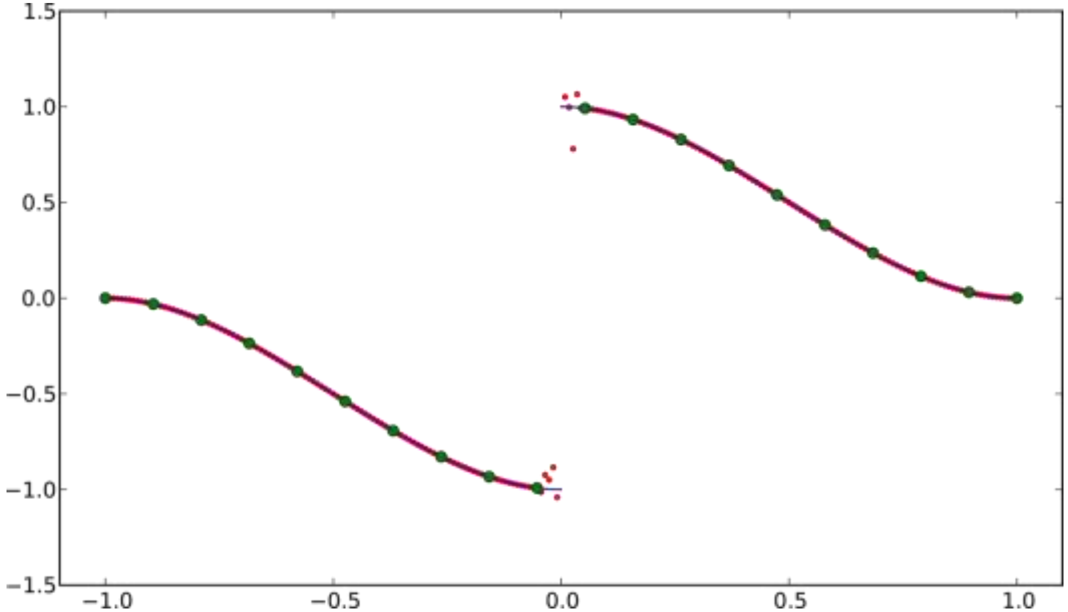


Moving Least Squares

Examples 1D

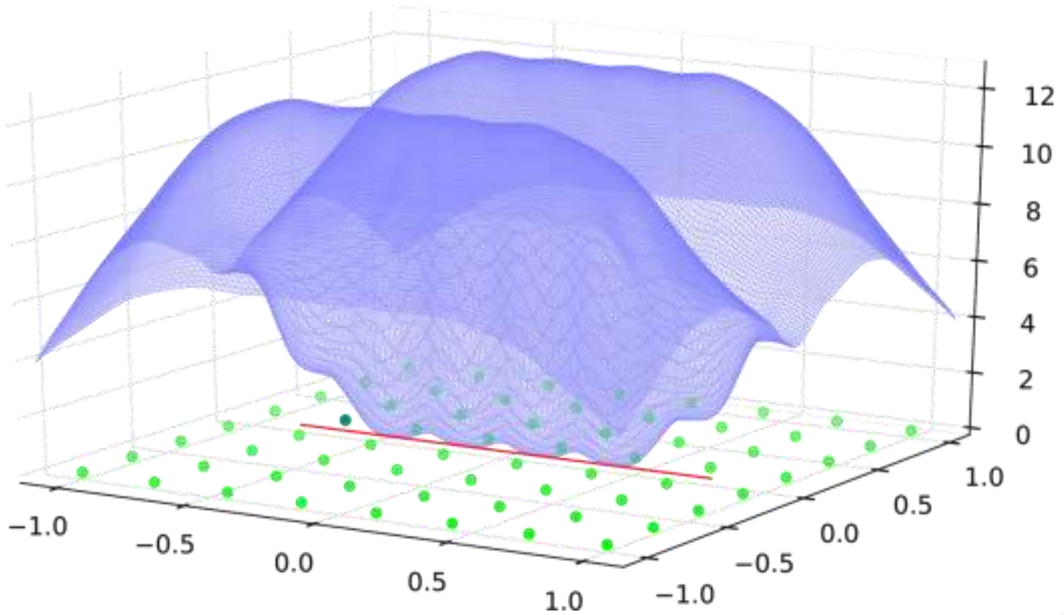


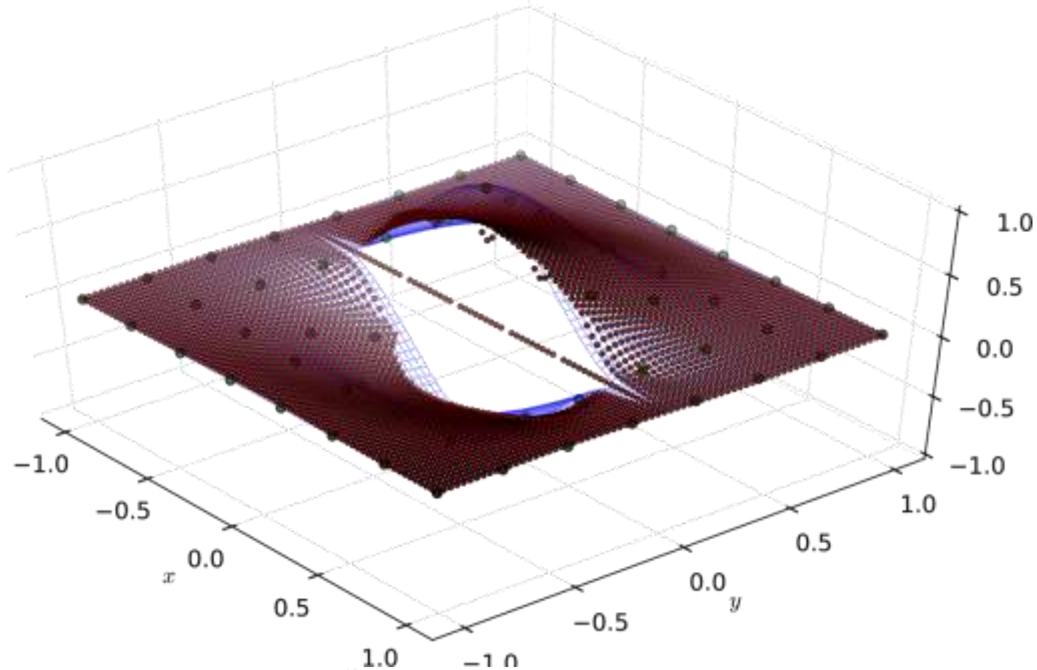


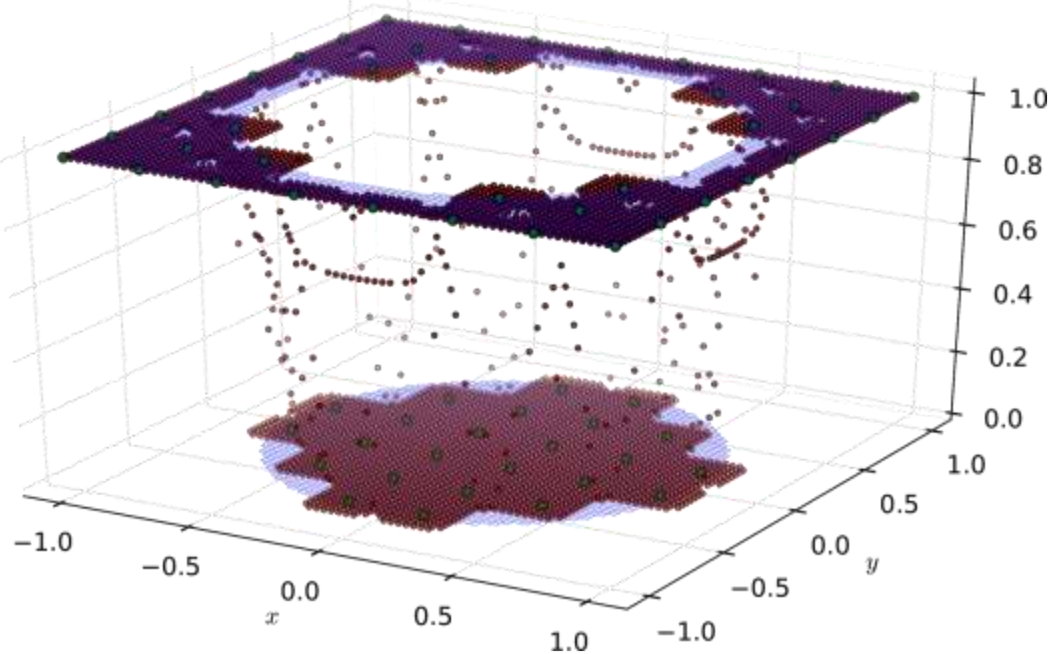


Moving Least Squares

Examples 2D

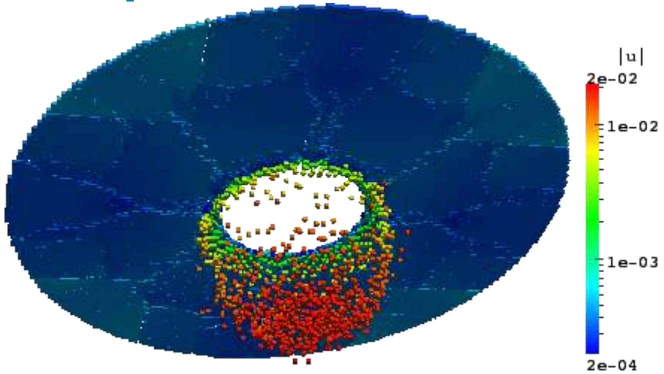




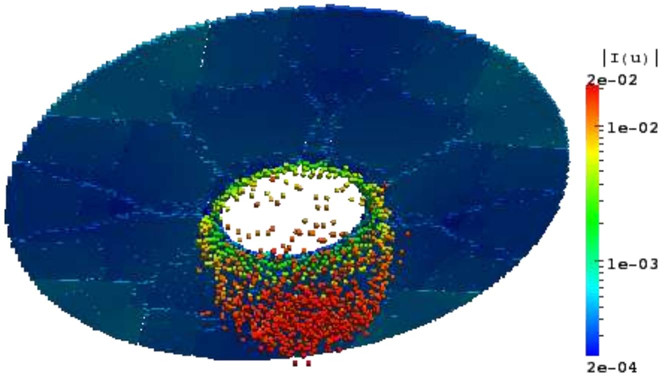


Moving Least Squares

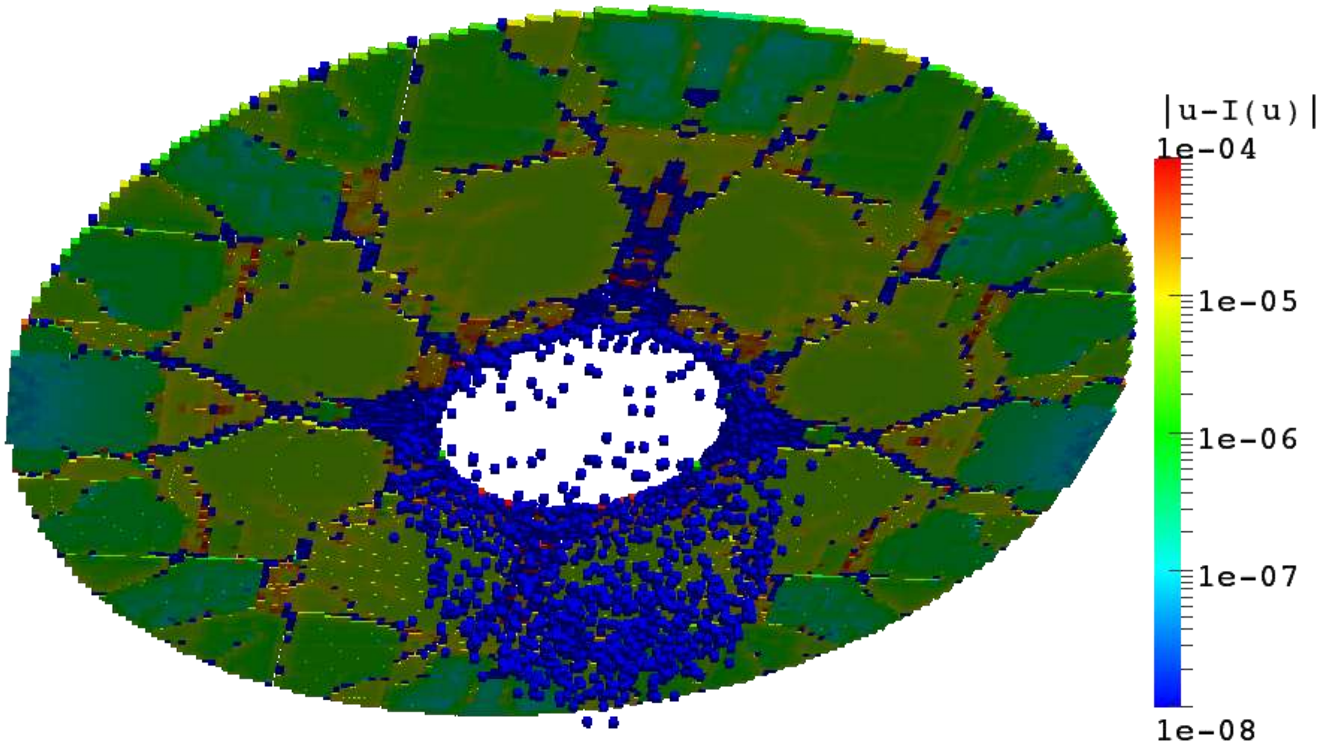
Example 3D



x+u

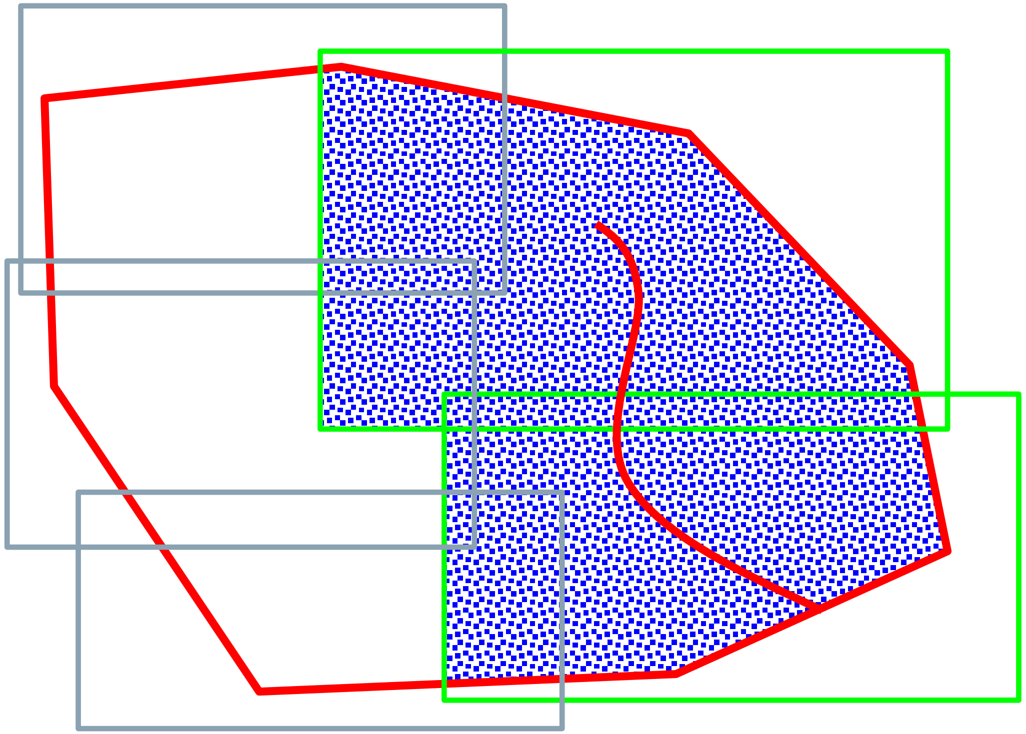


x+I(u)



approximation error

Idea



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Together

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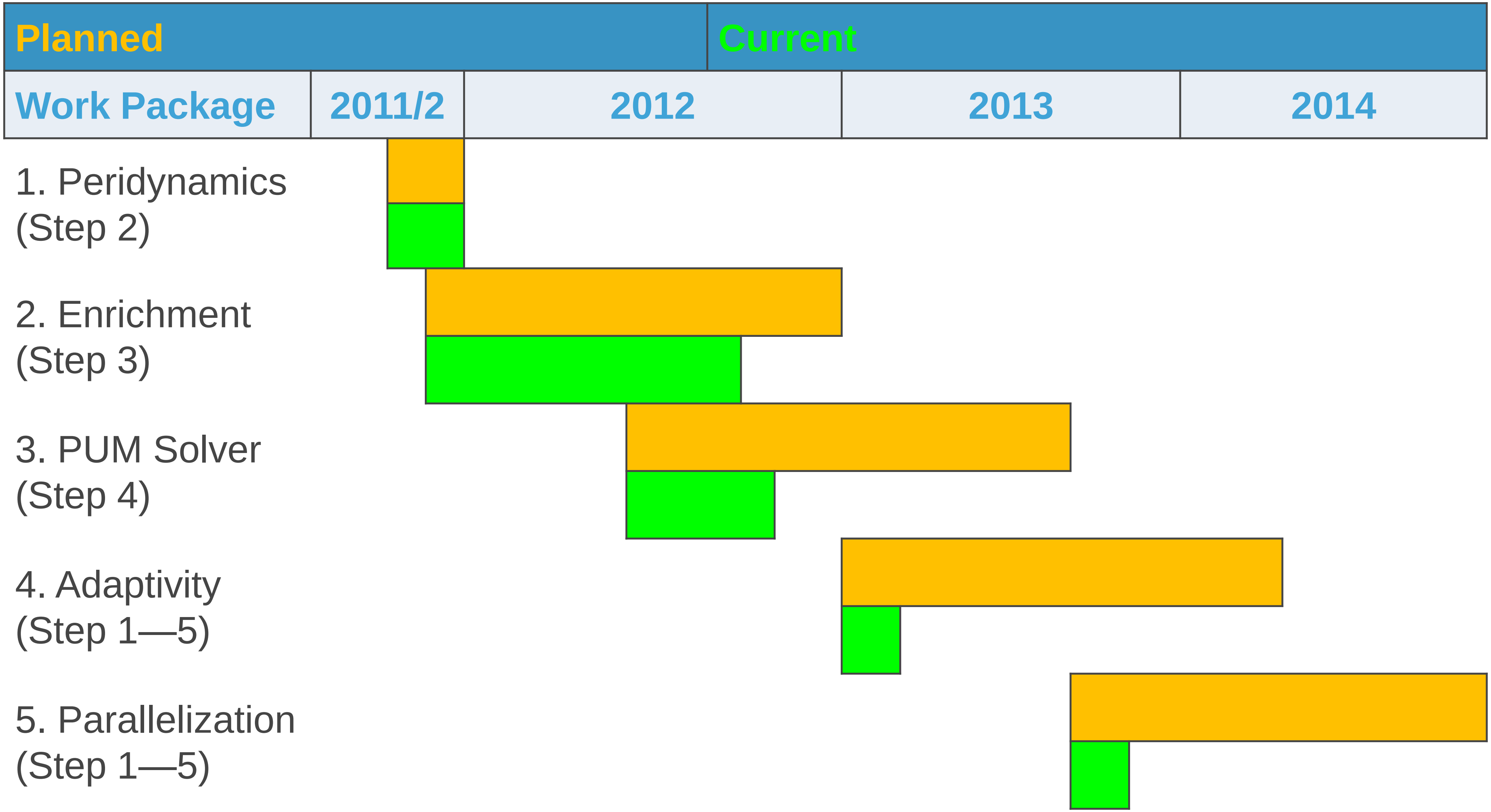
Project Status



Projections

2012

- Integration of MLS based enrichment
- Interpolation part of coupling

2013

- Full algorithmic cycle
- Early stages of Adaptivity
- Still looking for optimal components, parameters